

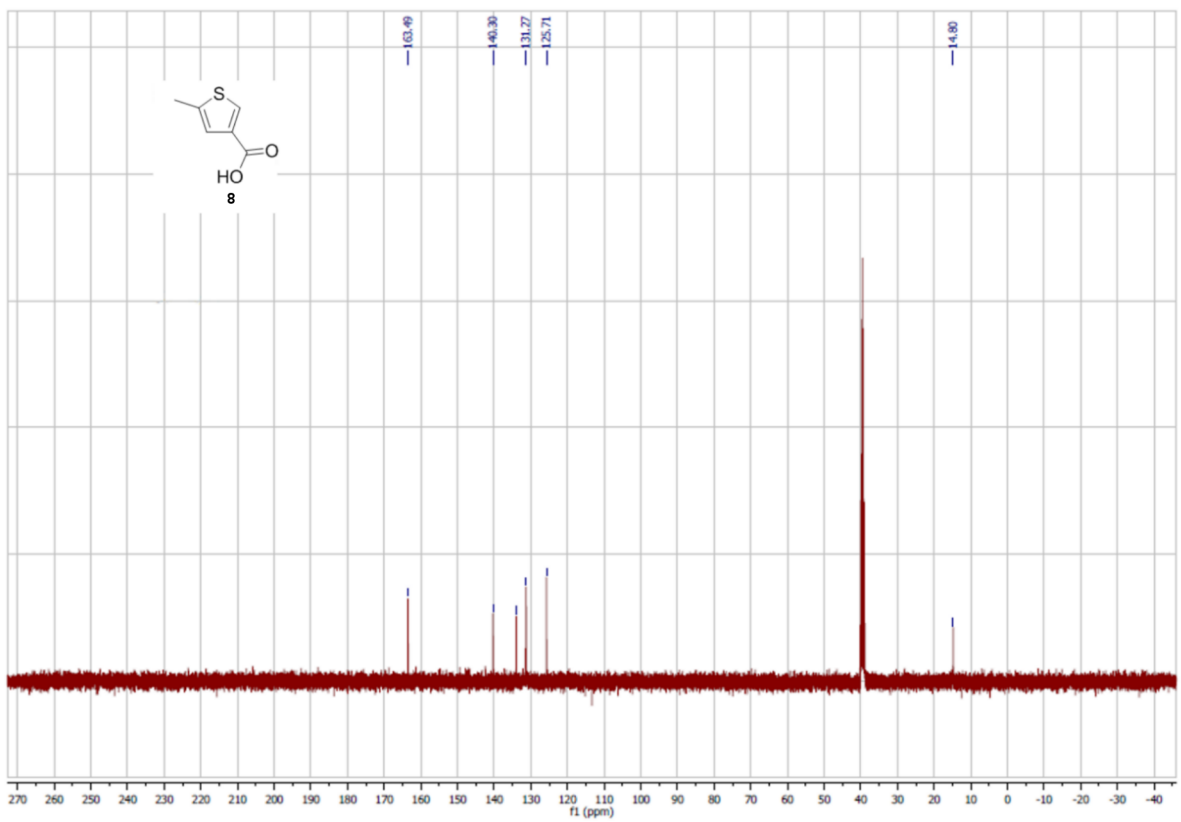
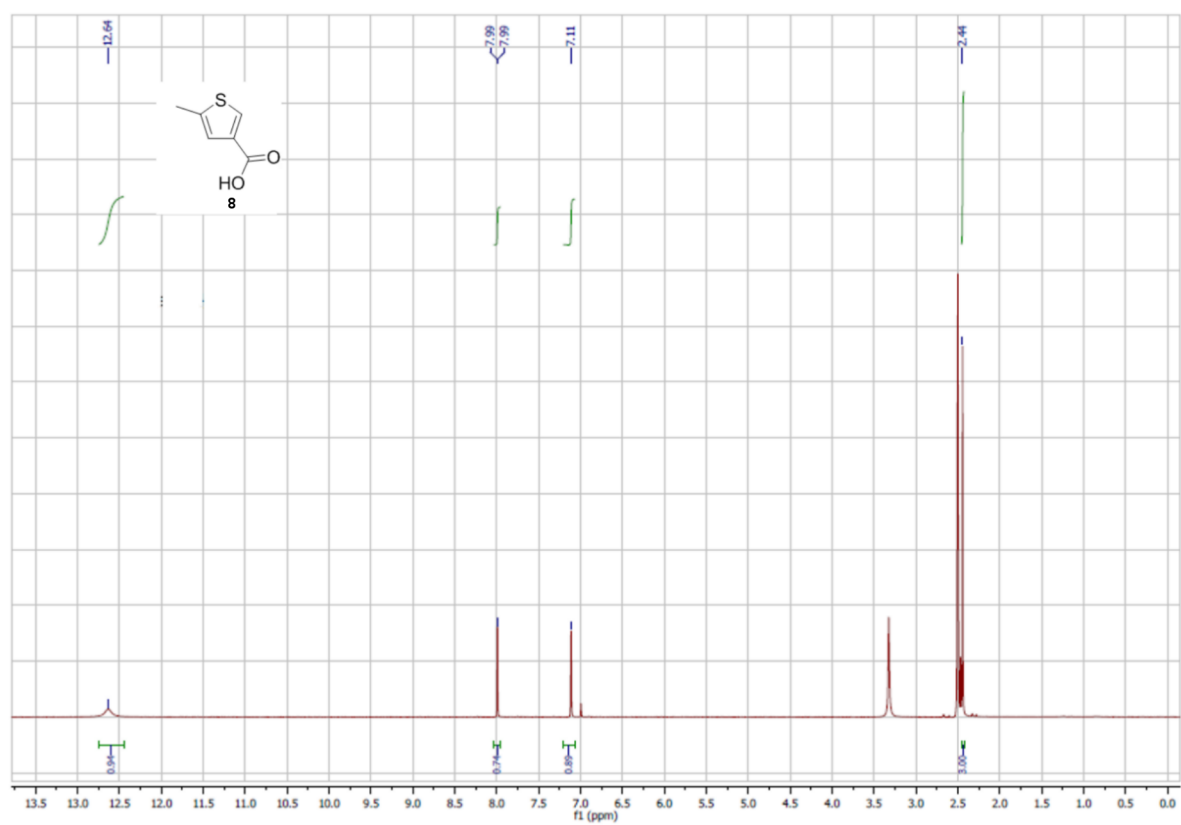
# **Furoates and Thenoates Inhibit Pyruvate Dehydrogenase Kinase 2 Allosterically by Binding to its Pyruvate Regulatory Site**

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Edelmiro Moman<sup>\*d,e</sup>

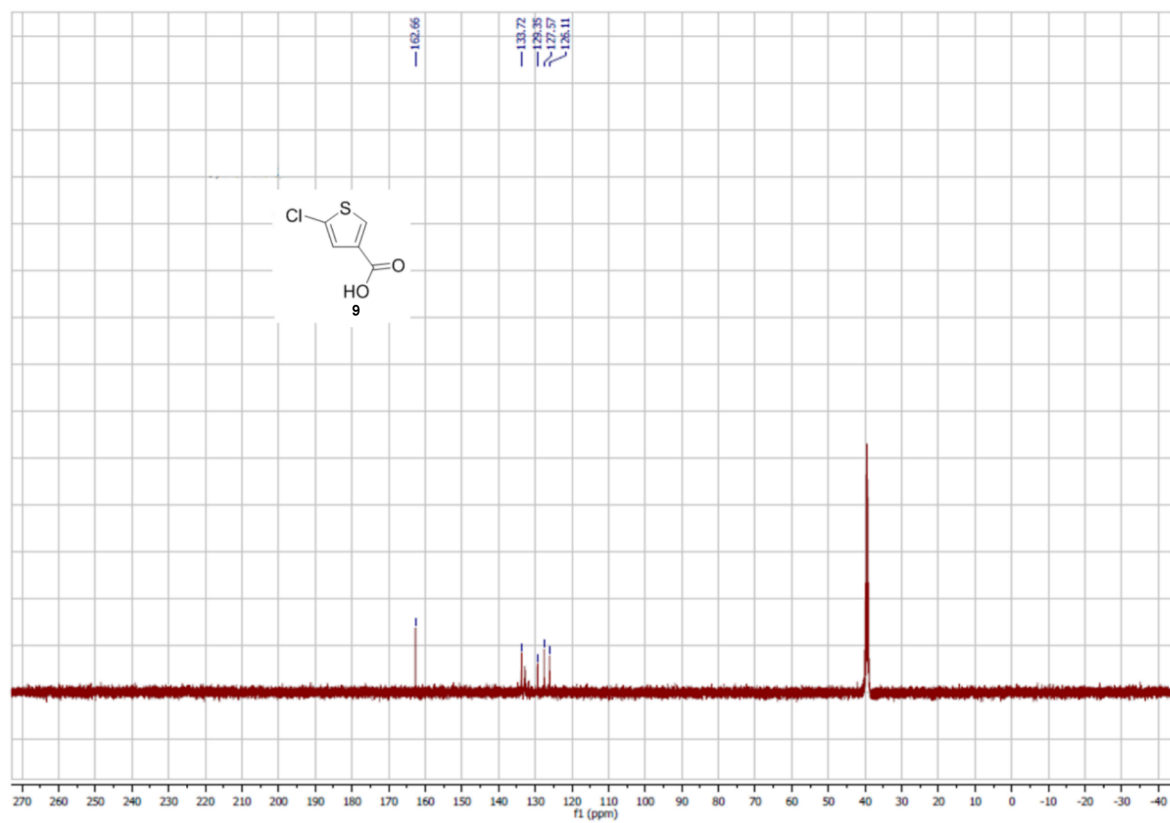
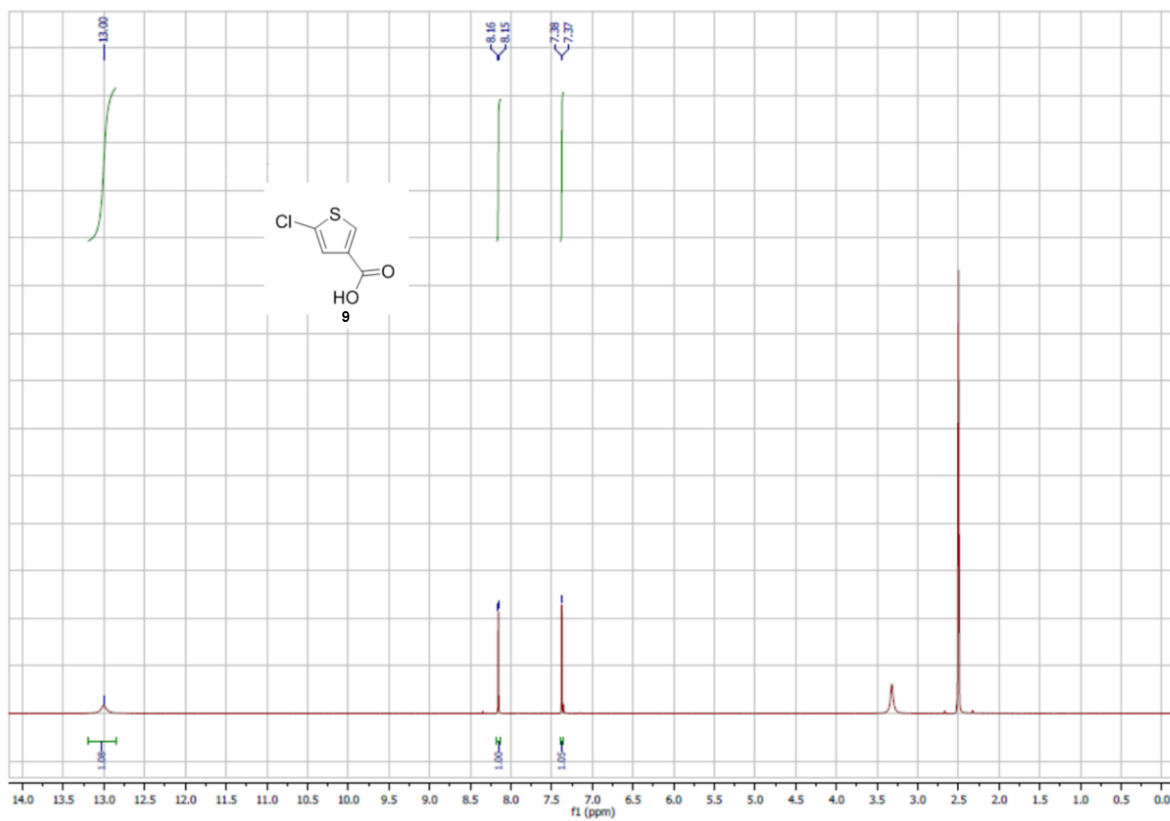
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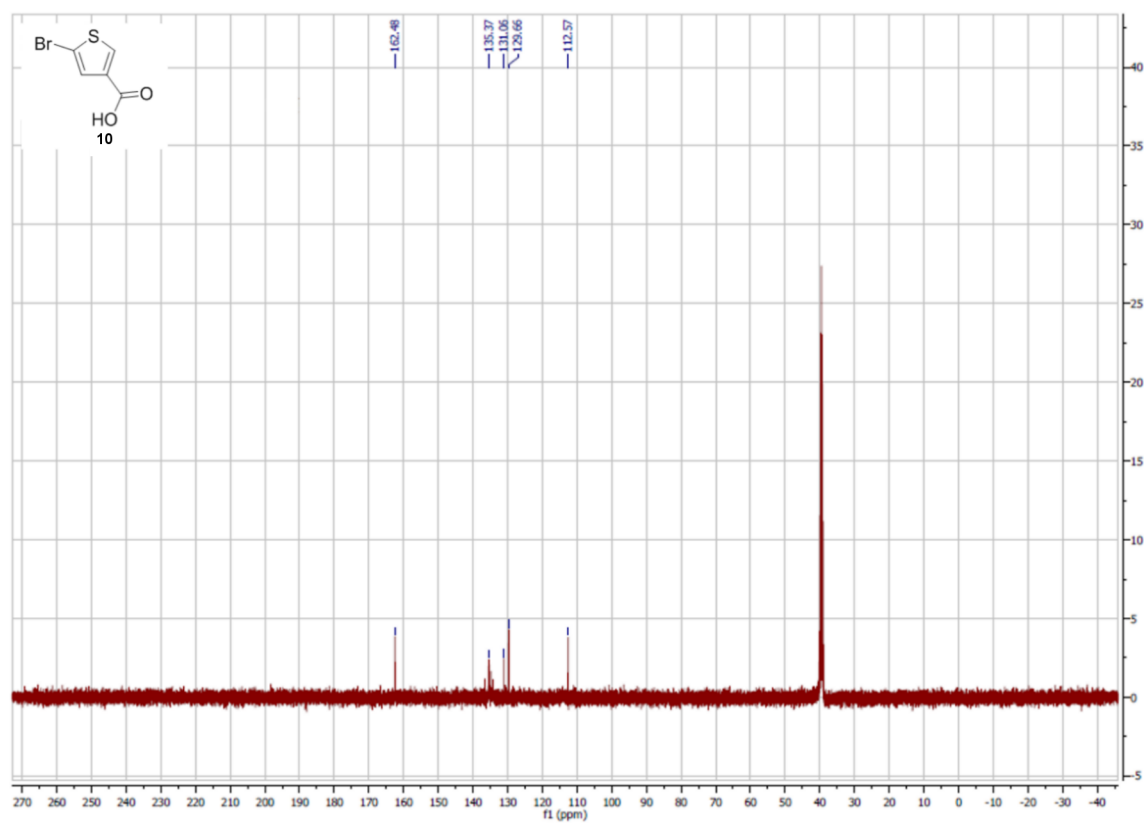
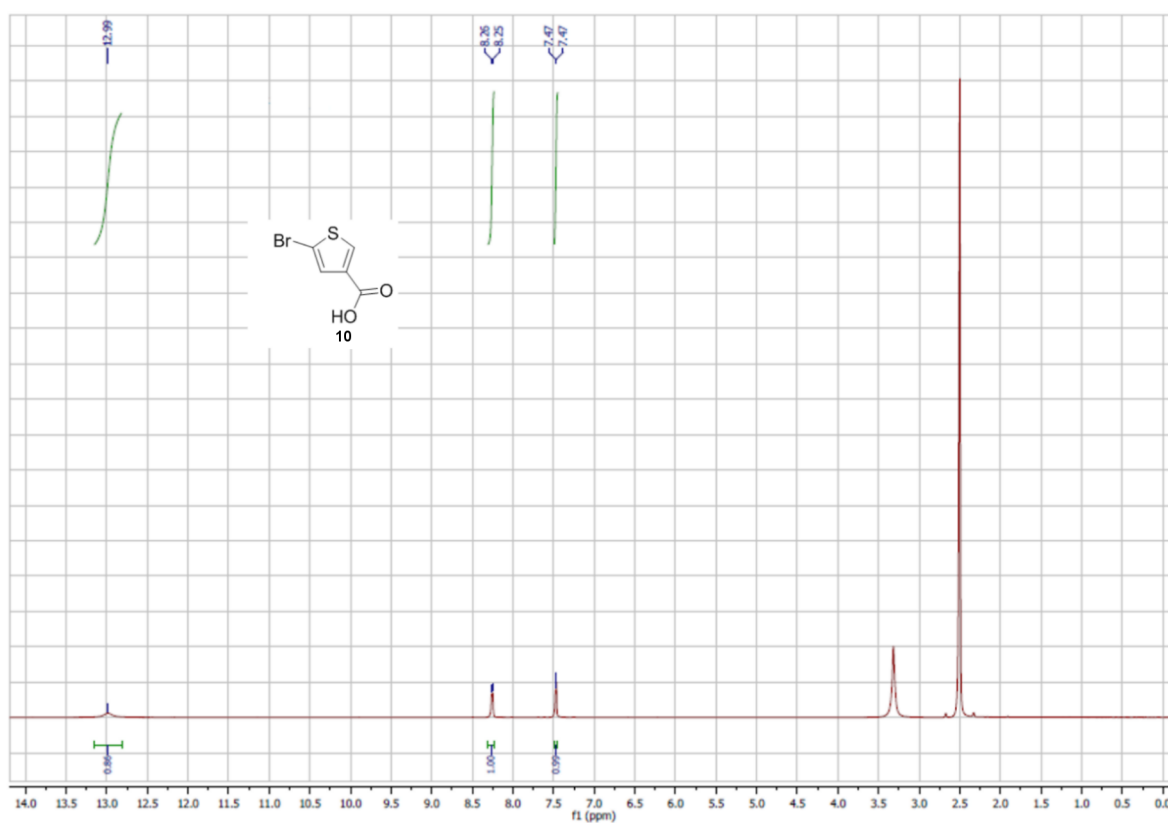
## **SUPPORTING INFORMATION**

- S1-S4**      <sup>1</sup>H-NMR and <sup>13</sup>C-NMR spectra of the synthesized compounds.
- S5-S10**    Inhibitor/PDK2 STD-NMR spectra.
- S11**        Inhibitor/DCA competition STD-NMR spectra.

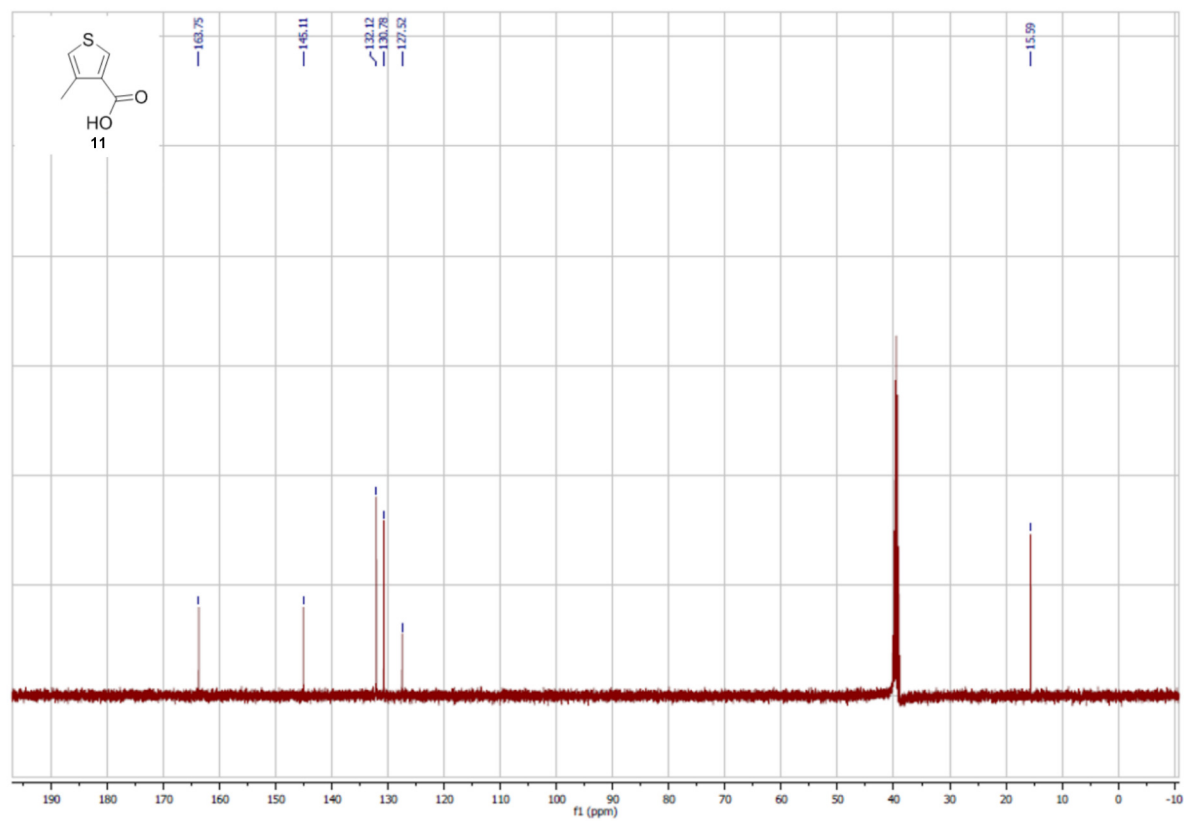
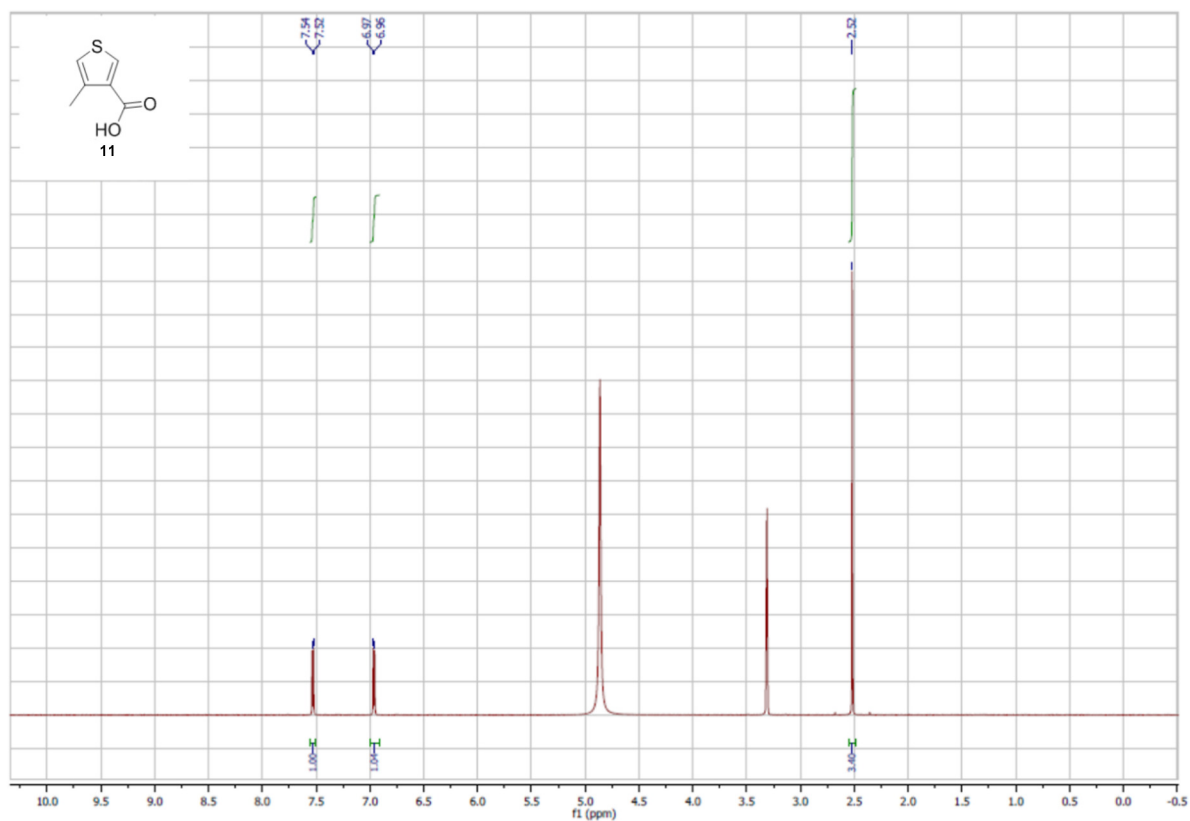


S1



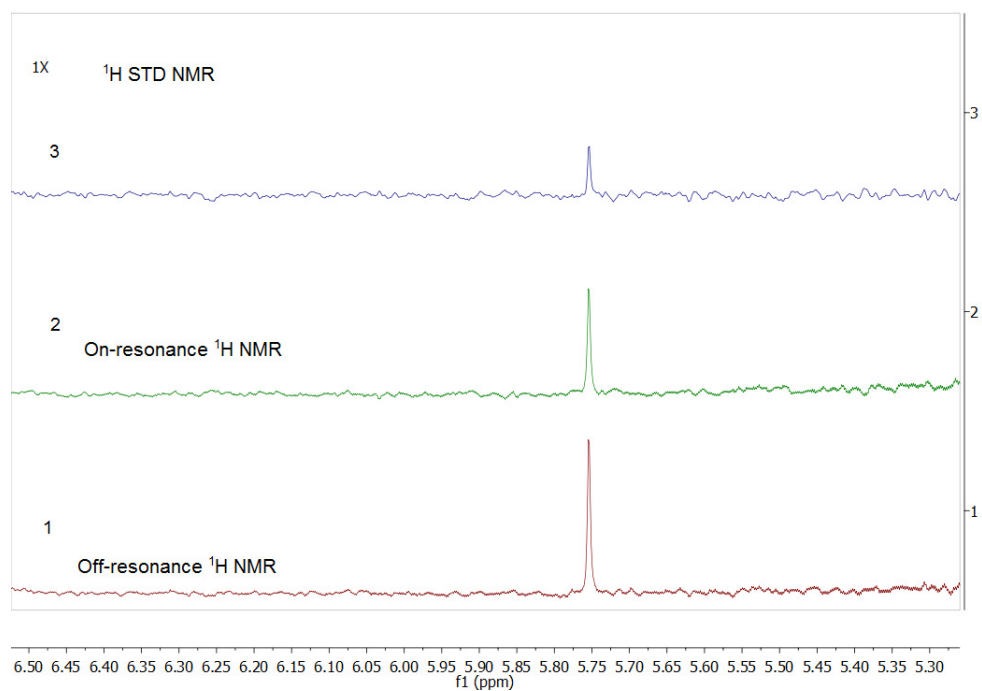


S3

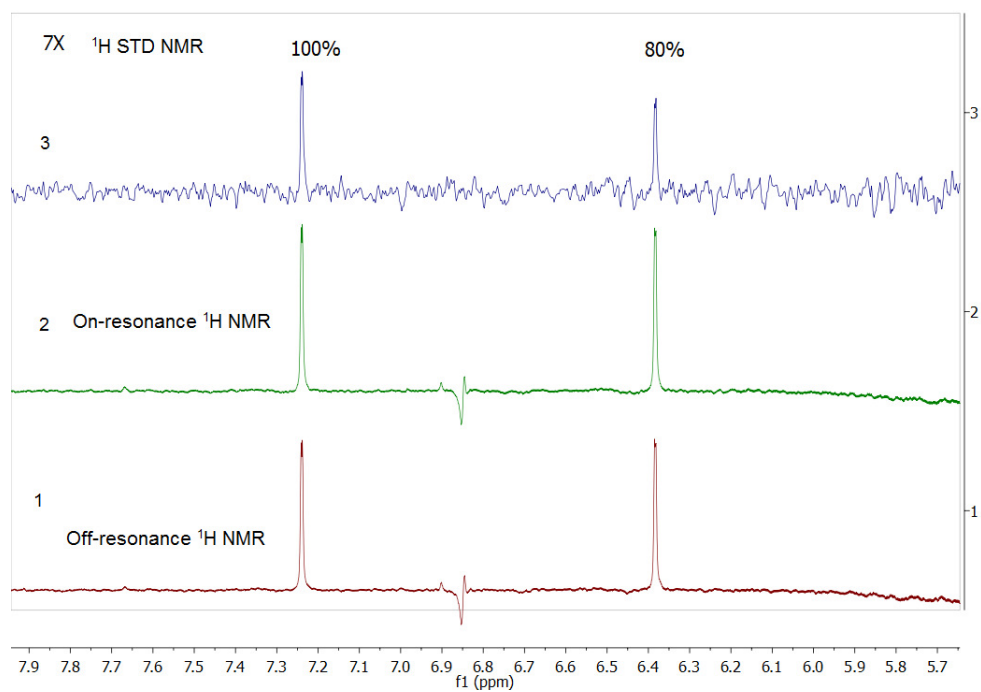


S4

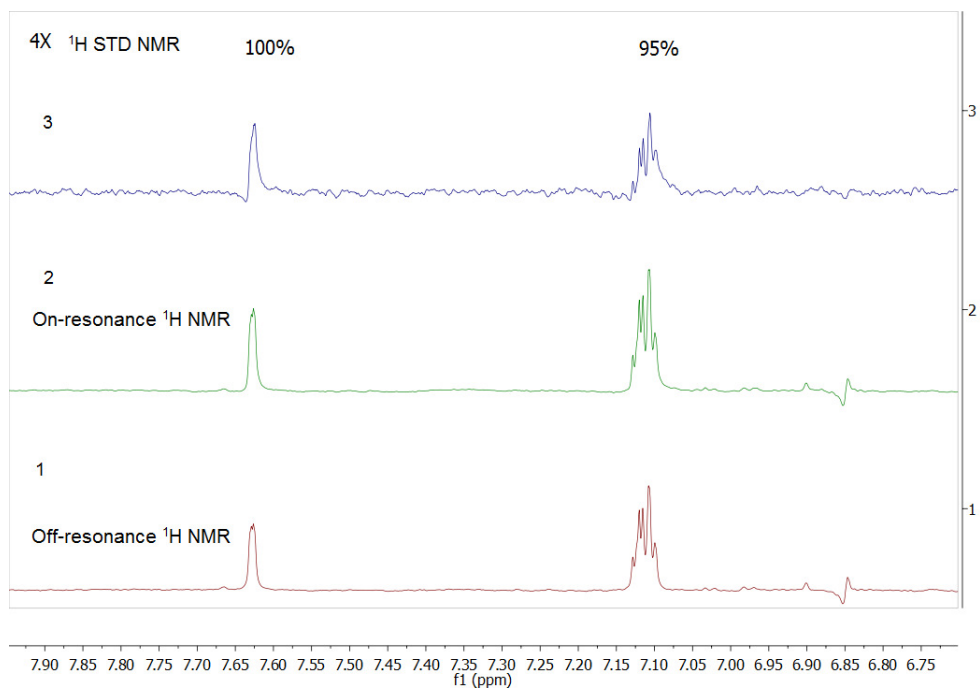
**Figure S5.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of DCA, 2) On-resonance  $^1\text{H}$ -NMR spectrum of DCA, 3)  $^1\text{H}$ -STD-NMR spectrum of DCA.



**Figure S6.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **4**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **4**, 3)  $^1\text{H}$ -STD-NMR spectrum of **4**.

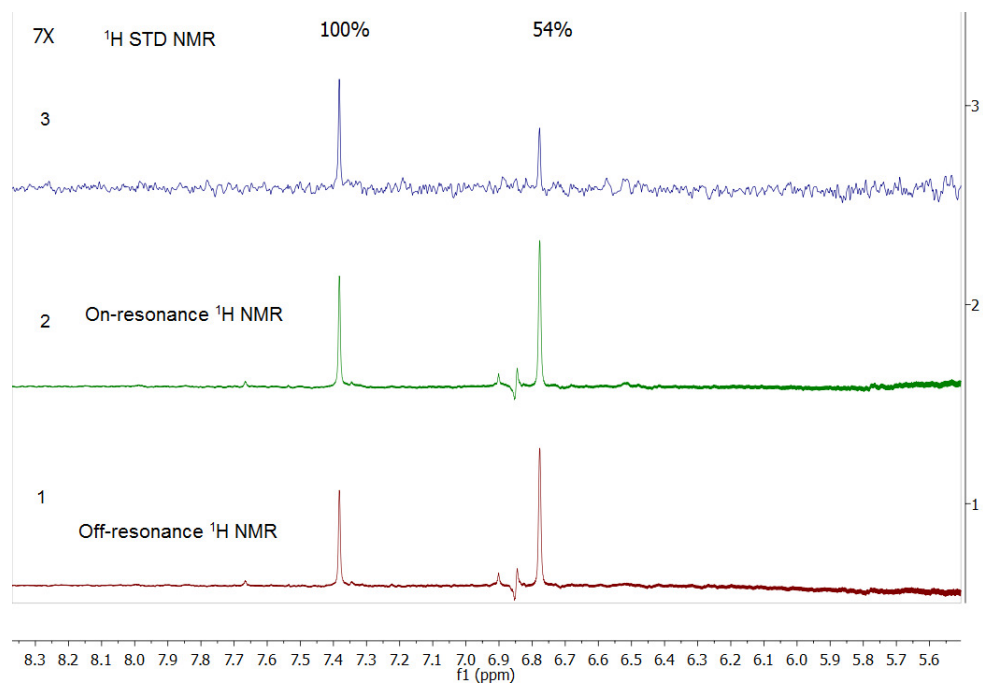


**Figure S7.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **5**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **5**, 3)  $^1\text{H}$ -STD-NMR spectrum of **5**. % Indicates the extend of interaction of specific protons with PDHK2.

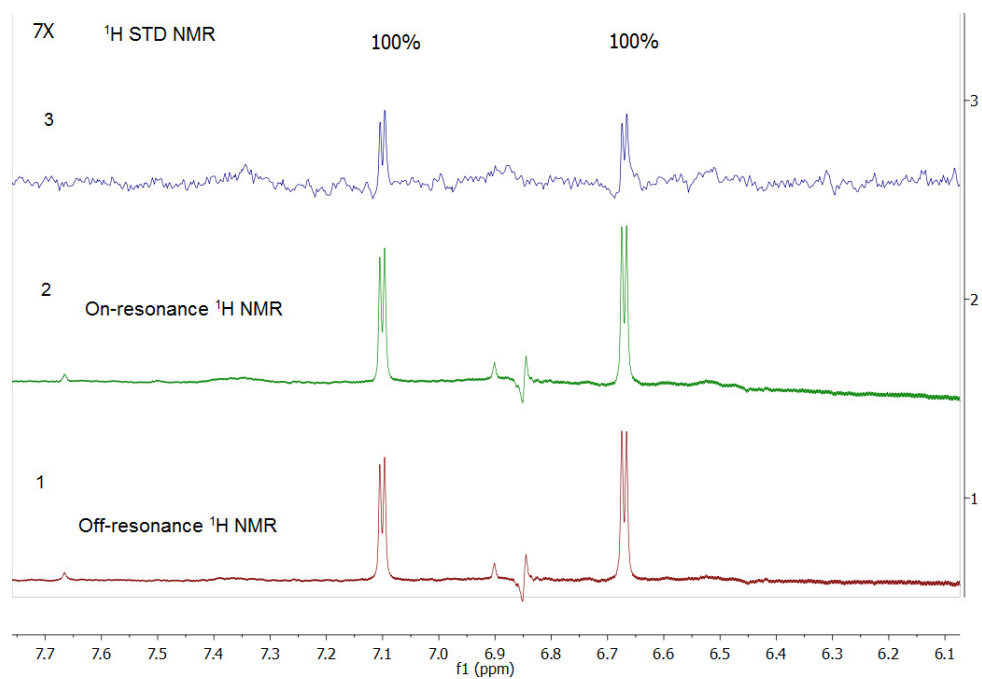




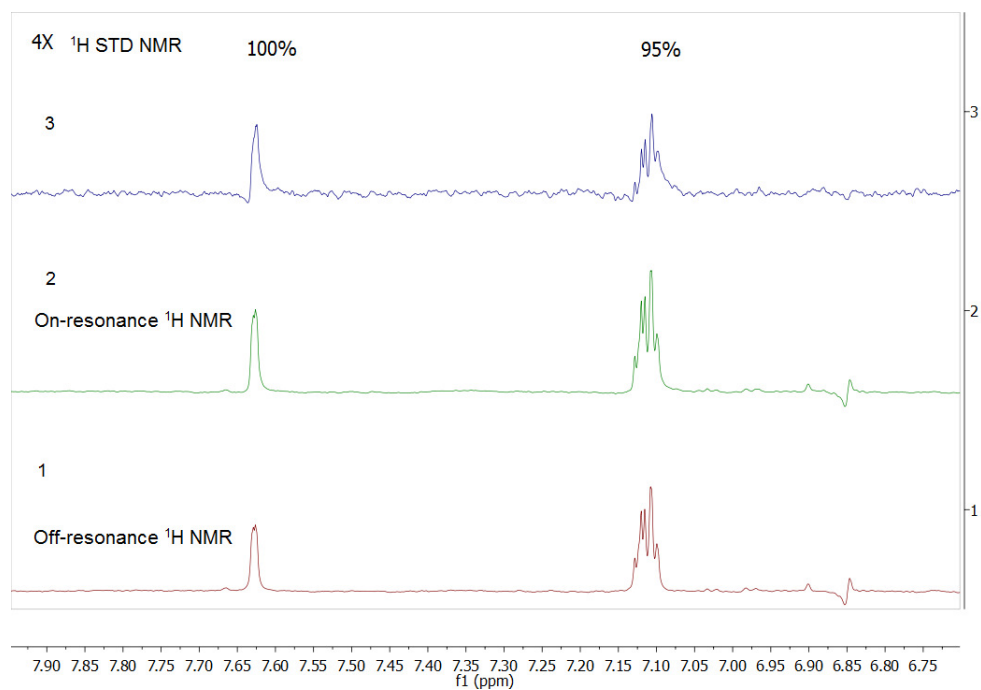
**Figure S8.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **8**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **8**, 3)  $^1\text{H}$ -STD-NMR spectrum of **8**.



**Figure S9.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **11**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **11**, 3)  $^1\text{H}$ -STD-NMR spectrum of **11**.



**Figure S10.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **12**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **12**, 3)  $^1\text{H}$ -STD-NMR spectrum of **12**. % Indicates the extend of interaction of specific protons with PDHK2.



**Figure S11.** 1) Off-resonance  $^1\text{H}$ -NMR spectrum of **8**, 2) On-resonance  $^1\text{H}$ -NMR spectrum of **8**, 3)  $^1\text{H}$ -STD-NMR spectrum of **8**, 4)  $^1\text{H}$ -STD-NMR spectrum of a mixture of **8** and **DCA**.

